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The Mie-Grüneisen Power Equation of State

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ABSTRACT

We describe details of a general Mie-Grüneisen equation of state and its numerical implementation. The equation of state contains a polynomial Hugoniot reference curve, an isentropic expansion and a tension cutoff.

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CONTENTS

TERMS AND DEFINITIONS

ρ_0 Reference state density

η Volumetric Strain

T_0 Reference state temperature

C_v Heat capacity at constant volume (assumed constant)

Γ Grüneisen parameter

α $\Gamma\rho_0/(1-\eta) = \Gamma\rho = \Gamma_0\rho_0$ (assumed constant)

C_0 Reference sound speed

$K_0 = \rho_0 C_0^2$ Reference adiabatic bulk modulus

K_n Hugoniot coefficient

P_{min} Minimum pressure on expansion isentrope

U_s Shock velocity in $U_s - u_p$ shock relationship

u_p Particle velocity in $U_s - u_p$ shock relationship

s Linear coefficient in $U_s - u_p$ shock relationship

ρ Density

P Pressure

E Specific internal energy

T Temperature

S Entropy

C_s Sound speed, $\sqrt{(\partial P/\partial \rho)_S}$

1. THE MIE-GRÜNEISEN POWER EQUATION OF STATE

1.1. INTRODUCTION

The classical Mie-Grüneisen equation of state assumes that the pressure is non-linearly related to the density but linear in the specific energy relative to a reference curve, R. Thus

$$P(\eta, E) = P_R(\eta) + \alpha \left[E - E_R(\eta)\right] \tag{1.1}$$

where the volumetric strain η is

$$\eta = 1 - \frac{\rho_0}{\rho} = 1 - \frac{v}{v_0}. \tag{1.2}$$

ρ is the density and v is the specific volume. The subscript 0 refers to a particular point on the reference curve where the strain is zero and the pressure is zero. This point is called the reference state. In addition, we assume that $\alpha = \Gamma\rho_0/(1-\eta) = \Gamma\rho = \Gamma_0\rho_0$ is constant. Γ is the Grüneisen parameter. The heat capacity $C_v = (\partial E/\partial T)_v$ is also assumed constant giving

$$E(\eta, T) = E_R(\eta) + C_v \left[T - T_R(\eta)\right] \tag{1.3}$$

Historically, the Mie-Grüneisen equation of state has been primarily used with application to compression of metal solids [2] and the compressive reference curve is assumed to be a Hugoniot. However, the reference curve can be a different curve. For example, a Mie-Grüneisen equation of state using a reference isentrope was matched to a Mie-Grüneisen $U_s - U_p$ shock Hugoniot with two parameters for the purpose of demonstrating relevant two dimensional isentropic jet flows [3].

The sound speed is computed by differentiating Equation 1.1 with respect to density at constant entropy and utilizing the thermodynamic relationship

$$dE = TdS - Pdv = TdS + Pv^2 d\rho. \tag{1.4}$$

Thus

$$\begin{aligned} C_s^2 = \left(\frac{\partial P}{\partial \rho}\right)_S &= P_R'(\eta)\frac{d\eta}{d\rho} + \alpha\left(\left(\frac{\partial E}{\partial \rho}\right)_S - E_R'(\eta)\frac{d\eta}{d\rho}\right) \\ &= v^2\left[\rho_0 P_R'(\eta) + \alpha\left(P - \rho_0 E_R'(\eta)\right)\right] \end{aligned} \tag{1.5}$$

since $d\eta/d\rho = \rho_0 v^2$. In addition,

$$\left(\frac{\partial P}{\partial \rho}\right)_T = v^2\rho_0\left[P_R'(\eta) - \alpha C_v T_R'(\eta)\right] \tag{1.6}$$

We now derive a useful and well known thermodynamics relation for integrating temperature along the references curves [4, Equation 23]. First,

$$\begin{aligned} dS &= \frac{1}{T}dE + \frac{P}{T}dv && (1.7)\\ &= \frac{1}{T}\left(\frac{\partial E}{\partial T}\right)_v dT + \frac{1}{T}\left(\left(\frac{\partial E}{\partial v}\right)_T + P\right)dv && (1.8)\\ &= \left(\frac{\partial S}{\partial T}\right)_v dT + \left(\frac{\partial S}{\partial v}\right)_T dv && (1.9) \end{aligned}$$

The equality of mixed differentials leads to

$$\left(\frac{\partial E}{\partial v}\right)_T + P = T\left(\frac{\partial P}{\partial T}\right)_v \tag{1.10}$$

and finally

$$T\,dS = C_v dT + T\left(\frac{\partial P}{\partial T}\right)_v dv \tag{1.11}$$

For the Mie-Grüneisen equation of state with constant C_v and constant $\alpha = \rho\Gamma = \rho_0\Gamma_0$, we then derive

$$T\,dS = C_v dT - \Gamma_0 C_v T\,d\eta \tag{1.12}$$

Equation 1.12 is the key thermodynamic relationship used below to compute the temperature along the reference curve.

The general Mie-Grüneisen power series equation of state described here contains polynomial flexibility in the shape of the reference curves. The subscript R refers to a reference state curve which is either a Hugoniot (subscript H) or an isentrope (subscript I). This particular model provides three regions: a compressive region, a tension region, and a tensile pressure cutoff region as described below.

1.2. COMPRESSION

For $\eta > 0$ we define:

$$P_R = P_H = K_0\eta\left(1 + K_1\eta + K_2\eta^2 + K_3\eta^3 + \cdots + K_M\eta^M\right) \tag{1.13}$$

where M is an integer giving the maximum number of terms in the polynomial and the subscript H indicates that the reference curve is a Hugoniot. The first term, $K_0 = \rho_0 C_0^2$, defines the adiabatic bulk modulus at the reference point.

The energy on the Hugoniot curve is given by the well-known shock jump conditions [1]

$$E_R = E_H = \frac{P_H \eta}{2\rho_0} + E_0. \tag{1.14}$$

In order to compute the temperature on the Hugoniot, we use the method of Walsh and Christian valid for constant $\alpha = \rho\Gamma$ and constant C_v [4]. This method uses Equationn 1.14 and Equation 1.12 to obtain the temperature on the Hugoniot curve,

Substituting Equation 1.12 on the left hand side of Equation 1.7 and the shock jump condition Equation 1.14 on the right hand side, we obtain a differential equation for the temperature along the Hugoniot curve,

$$C_v \frac{dT_H}{d\eta} - \Gamma_0 C_v T_H = \frac{dE_H}{d\eta} - v_0 P_H = \frac{v_0 \eta^2}{2} \frac{d}{d\eta}\left(\frac{P_H}{\eta}\right). \tag{1.15}$$

Integration on the Hugoniot curve gives

$$T_H = T_0 e^{\Gamma_0 \eta} + \frac{e^{\Gamma_0 \eta}}{2C_v \rho_0} \int_0^\eta e^{-\Gamma_0 z} z^2 \frac{d}{dz}\left(\frac{P_H}{z}\right) dz \tag{1.16}$$

which leads to

$$T_H = T_0 e^{\Gamma_0 \eta} + \frac{e^{\Gamma_0 \eta}}{2C_v \rho_0} K_0 \left(K_1 I_2 + 2K_2 I_3 + 3K_3 I_4 + \cdots + MK_M I_{M+1}\right) \tag{1.17}$$

where

$$I_n = \int_0^\eta e^{-\Gamma_0 z} z^n dz \tag{1.18}$$

$$= \left(\frac{1}{\Gamma_0}\right)^{n+1} \int_0^{\Gamma_0 \eta} e^{-z} z^n dz \tag{1.19}$$

$$= \left(\frac{1}{\Gamma_0}\right)^{n+1} \gamma(n+1, \Gamma_0 \eta) \tag{1.20}$$

and

$$\gamma(n,x) = \int_0^x e^{-z} z^{n-1} dz \tag{1.21}$$

is the lower incomplete gamma function. The η derivative of T_H is

$$\frac{dT_H}{d\eta} = \Gamma_0 T_H + \frac{K_0}{2C_v \rho_0}\left(K_1 \eta^2 + 2K_2 \eta^3 + 3K_3 \eta^4 + \cdots + MK_M \eta^{M+1}\right) \tag{1.22}$$

We need to evaluate $\gamma(n,x)$ for arguments, $x \geq 0$, and integral $n \geq 3$. As a first cut one might think to use the well known formula

$$\gamma(n,x) = (n-1)!\left(1 - e^{-x} \sum_{k=0}^{n-1} \frac{x^k}{k!}\right) \tag{1.23}$$

$$= (n-1)!\left(1 - e^{-x} e_{n-1}(x)\right) \tag{1.24}$$

where $e_n(x)$ is the exponential sum function [5]. This identity can be shown by induction using integration by parts (integrate the exponential factor). This formula would seem to allow for efficient computation of the required M values of the lower incomplete gamma function. However, the factorial term multiplied by the difference of two terms that might be close in magnitude suggest that floating point precision could easily be lost as n increases. Numerical experiments confirmed this and the algorithm was deemed unsuitable.

However, one can use integration by parts on Equation 1.21 (integrating the polynomial factor), to derive

$$\gamma(n,x) = e^{-x}\sum_{k=0}^{N-1}\frac{x^{n+k}}{n(n+1)\cdots(n+k)} + \frac{1}{n(n+1)\cdots(n+N-1)}\int_0^x e^{-z}z^{n+N-1}dz \tag{1.25}$$

$$= S^N + E^N \tag{1.26}$$

where the sum S^N has N terms and E^N is the final integral term in Equation 1.25. A simple estimate gives

$$E^N \le \frac{x^{n+N-1}(1-e^{-x})}{n(n+1)\cdots(n+N-1)}. \tag{1.27}$$

An alternate notation is now convenient. If we define

$$\gamma_2(n,x) = x^{-n}e^x\gamma(n,x) \tag{1.28}$$

then

$$\gamma_2(n,x) = \sum_{k=0}^{N-1}\frac{x^k}{n(n+1)\cdots(n+k)} + \frac{e^x x^{-n}}{n(n+1)\cdots(n+N-1)}\int_0^x e^{-z}z^{n+N-1}dz \tag{1.29}$$

$$= S_2^N + E_2^N \tag{1.30}$$

Similarly, we have

$$E_2^N \le \frac{x^{N-1}e^x(1-e^{-x})}{n(n+1)\cdots(n+N-1)} \tag{1.31}$$

and to achieve double precision relative accuracy for $\gamma_2(n,x)$, we stop adding terms when

$$E_2^N \le 10^{-15}S_2^N. \tag{1.32}$$

We have also

$$e^{\Gamma_0\eta}I_n = \gamma_2(n+1,\Gamma_0\eta)\eta^{n+1} \tag{1.33}$$

which leads to the convenient form

$$T_H = T_0e^{\Gamma_0\eta} + \frac{K_0}{2C_v\rho_0}\sum_{i=1}^{M} iK_i\eta^{i+2}\gamma_2(i+2,\Gamma_0\eta) \tag{1.34}$$

Since we potentially have a large number of terms to evaluate, we look for even more efficiency by looking for a stable backward recurrence for γ_2 that will allow for computing $\gamma_2(n,x)$ at the same time that Equation 1.34 is evaluated as a telescoping sum.

Integrating by parts on Equation 1.21 (integrating the polynomial factor once), we derive

$$\gamma(n,x) = \frac{1}{n}\left(\gamma(n+1,x) + e^{-x}x^n\right) \tag{1.35}$$

and the corresponding recursion relation for γ_2 is

$$\gamma_2(n,x) = \frac{x}{n}\gamma_2(n+1,x) + \frac{1}{n}. \tag{1.36}$$

which is a backward recurrence with a starting value $\gamma_2(M+2,x)$ evaluated using Equation 1.29. Let $\varepsilon_2(n,x)$ be difference between the numerical solution and the exact solution for γ_2. This error satisfies the backward recurrence relation

$$\varepsilon_2(n,x) = \frac{x}{n}\varepsilon_2(n+1,x) \tag{1.37}$$

with solution

$$\varepsilon_2(n,x) = \frac{x^{M+2-n}}{n(n+1)(n+2)\cdots(M+1)}\varepsilon_2(M+2,x), \;\; 3 \le n \le M+1 \tag{1.38}$$

Utilizing Equation 1.24 to switch to a relative error ε_2^r, we obtain

$$\varepsilon_2^r(n,x) = \left(\frac{1-e^{-x}e_{M+1}(x)}{1-e^{-x}e_{n-1}(x)}\right)\varepsilon_2^r(M+2,x), \;\; 3 \le n \le M+1 \tag{1.39}$$

and it is seen that the backwards recurrence algorithm is stable and has a well controlled error. As a check, numerical results from the recurrence algorithm were compared to a direct evaluation of Equation 1.29. The numerical stability of recurrence relations has an extensive literature [6].

As an example of the power series form for the Hugoniot, we can compute the power series expansion of the linear $U_s - u_p$ Hugoniot in terms of η. The relevant shock jump equations are, respectively, mass, momentum conservation and the assumed linear $U_s - U_p$ relation:

$$\rho_0 U_s = \rho(U_s - u_p), \tag{1.40}$$

$$P_H = \rho U_s u_p \tag{1.41}$$

and

$$U_s = C_0 + s u_p \tag{1.42}$$

where U_s is the shock speed, C_0 is the sound speed at the initial (reference) state, s is the linear coefficient and u_p is the particle velocity. Eliminating U_s from Equation 1.40 results in

$$u_p = \frac{C_0\eta}{1-s\eta} \tag{1.43}$$

and substitution of Equation 1.42 and then Equation 1.43 in Equation 1.41 gives the Hugoniot entirely in terms of η

$$P_H = \frac{\rho_0 C_0^2 \eta}{(1-s\eta)^2} \tag{1.44}$$

Expanding Equation 1.44 in a power series in η results in

$$\begin{aligned} P_H &= \rho_0 C_0^2 \eta (1 + s\eta + (s\eta)^2 + (s\eta)^3 + \cdots)^2 && (1.45) \\ &= \rho_0 C_0^2 \eta (1 + 2s\eta + 3(s\eta)^2 + 4(s\eta)^3 + \cdots) && (1.46) \end{aligned}$$

so that $K_n = (n+1)s^n$ for $n \ge 1$.

1.3. EXPANSION

For $\eta_{min} = \frac{P_{min}}{K_0} \leq \eta < 0$, the reference curve is defined by an isentrope with a single fixed K_0.

$$P_R = P_I = K_0 \eta \tag{1.47}$$

Equation 1.7 in the form

$$\frac{dE}{d\eta} = v_0 P \tag{1.48}$$

yields

$$E_R = E_I = \frac{K_0 \eta^2}{2\rho_0} + E_0 \tag{1.49}$$

and Equation 1.12 in the form

$$\frac{dT}{d\eta} = \Gamma_0 T \tag{1.50}$$

results in

$$T_R = T_I = T_0 e^{\Gamma_0 \eta} \tag{1.51}$$

1.4. PRESSURE CUTOFF IN TENSION

Similarly, for $\eta < \eta_{min} = \frac{P_{min}}{K_0}$, we define a continuation of the isentropic reference curve which does not sustain additional tensile pressure. Thus

$$P_R = P_I = P_{min} \tag{1.52}$$

$$E_R = E_I = \frac{K_0 \eta_{min}^2}{2\rho_0} + E_0 + \frac{P_{min}}{\rho_0}(\eta - \eta_{min}) \tag{1.53}$$

$$T_R = T_I = T_0 e^{\Gamma_0 \eta} \tag{1.54}$$

1.5. CONCLUSION

We have documented details of a Mie-Grüneisen equation of state with a polynomial power series compressive Hugoniot reference curve and a linear isentropic expansion reference curve with a pressure cutoff in tension. A constant $\rho\Gamma$ product and constant heat capacity is assumed. The numerical approaches utilized in the evaluating the analytic solution are fully described.

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